

Orthoformic acid, cyclic 2,2-dimethyltrimethylene ethyl ester
5783-79-9 | DTXSID20206542

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.45

Global applicability domain: Inside

Local applicability domain index: 9.86e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,3-Dichlorobenzene</div> <div>Measured: 4.12</div> <div>Predicted: 4.44</div>	<div>Image not found</div> <div>1,4-Dichlorobenzene</div> <div>Measured: 4.46</div> <div>Predicted: 4.45</div>	<div>Image not found</div> <div>1,2-Dichlorobenzene</div> <div>Measured: 4.36</div> <div>Predicted: 4.46</div>
<div>Image not found</div> <div>Propylbenzene</div> <div>Measured: 4.09</div> <div>Predicted: 4.53</div>	<div>Image not found</div> <div>Octanal</div> <div>Measured: 5.36</div> <div>Predicted: 4.54</div>	